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Wave-Space Representation of the Electron Entropy in the Tight-Binding Approximation

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Abstract

The wave-space expression for the electron entropy averaged with respect to the hard-sphere reference system is obtained in the framework of the tight-binding model.

Keywords: Tight-binding model, electron entropy, wave space

The electron contribution to the entropy of a metal is expressed as follows (hereafter, in atomic units per atom):

$$S_e = (\pi k_b)^2 T n(\varepsilon_{\mathrm{F}})/3 \quad , \tag{1}$$

where ε_F is the Fermi energy, k_b - Boltzmann constant, T - temperature, $n(\varepsilon)$ - density of electron states.

The average of S_e with respect to the hard-sphere (HS) reference system is

$$\langle S_e \rangle_{HS} = (\pi k_b)^2 T \langle n(\varepsilon_F) \rangle_{HS} /3 \quad . \tag{2}$$

In the framework of the tight-binding model [1, 2]

$$\langle n(\varepsilon_F) \rangle_{HS} = 10 \sqrt{\frac{1}{2\pi\mu_{HS}}} e^{-\frac{\varepsilon_F^2}{2\mu_{HS}}} \quad , \tag{3}$$

where

$$\mu_{HS} = 4\pi\rho \int_0^\infty \beta^2(r) g_{HS}(r) r^2 \mathrm{d}r \quad . \tag{4}$$

Here, $g(r)$ is the radial distribution function, ρ - mean atomic density,

$$\beta(r) = B\exp(-br) \quad , \tag{5}$$

where B and b are parameters.

In [2] was found that the magnitude of $e^{-\frac{\varepsilon_F^2}{2\langle\mu_m\rangle_{HS}}}$ is a constant for each metal since it depends on the number of *d* electrons per atom, N_d , only. As a result, Eq. (3) can be rewritten by the following way:

$$\langle n(\varepsilon_F)\rangle_{HS} = 10\sqrt{\frac{1}{2\pi\mu_{HS}}}\, f(N_d) \tag{6}$$

To convert Eq. (2) to the wave space we use the relation

$$g(r) = 1 + \frac{1}{2\rho\pi^2}\int_0^\infty [S(q)-1]\frac{\sin(qr)}{qr}q^2\mathrm{d}q \quad , \tag{7}$$

where $S(q)$ is the structure factor.

After Fourier transform we obtained the following expression:

$$\langle S_e\rangle_{HS} = \frac{10}{\sqrt{2\pi}} f(N_d)\frac{(\pi k_b)^2 T}{3\sqrt{\tilde{\mu}_{HS}}} \quad , \tag{8}$$

where

$$\tilde{\mu}_{HS} = \frac{\pi\rho B^2}{b^3} + \frac{8bB^2}{\pi}\int_0^\infty (S_{HS}(q)-1)\left[\frac{q}{(4b^2+q^2)}\right]^2 \mathrm{d}q \quad . \tag{9}$$

References

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